Quantum Mechanics

TOPIC: Quantum Numbers

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Introduction

- The Quantum Theory helps describe how electrons are organized in the atom by using 4 distinct numbers. They help to describe where electrons are most likely to be found.

1. Principal Quantum Number (n)
2. Angular-momentum quantum Number (l)
3. Magnetic Quantum Number (M_l)
4. Magnetic Spin (M_s)

1. Principal Quantum Number (n)

The Principal Quantum Number is always a positive number which is dependant on the size of the atom and energy level. As the number of orbitals increases the value of n becomes larger. In turn, the distance between the electrons and the nucleus become farther apart. Since it takes energy to separate a negative charge from a positive charge, the increased distance between the nucleus and the electron means that the energy of the electron increases along with the Principal Quantum Number.

2. Angular-momentum Number (l)

This is the number that defines the dimensional shape of the orbital. Orbitals are grouped into different subshells/levels, these are classified under the following groups s, p, d, f.

For example:

$l = 0$ then it has the shape of a Sphere $\longrightarrow$ s

$l = 1$ then it has the shape of a Dumbell $\longrightarrow$ p

$l = 2$ then it has Various Shapes $\longrightarrow$ d

$l = 3$ then it has Various Shapes $\longrightarrow$ f

$l = 4$ then it has Various Shapes $\longrightarrow$ g

3. Magnetic Quantum Number (M_l)

This number describes which orbital an electron is most likely to be found. If an orbital that has an angular-momentum number of 1, the magnetic quantum numbers can have any integral number from -1 to 1.

For Example:

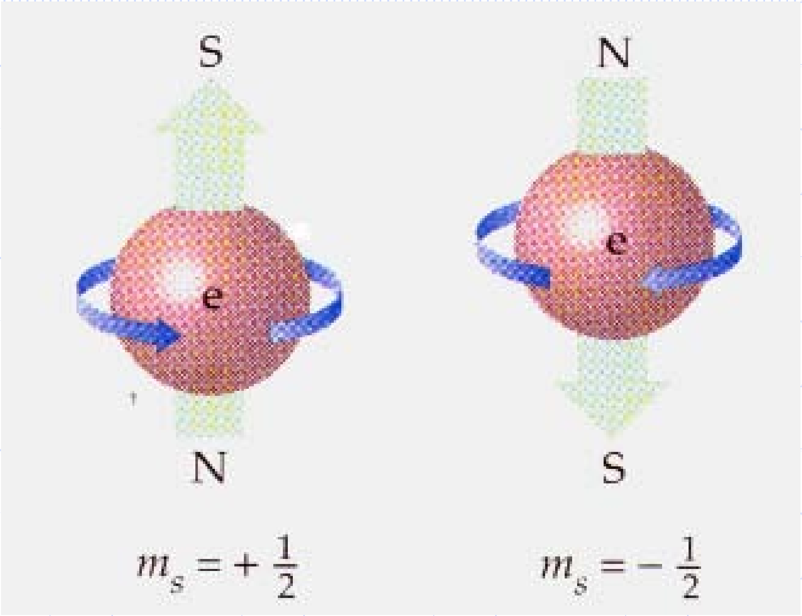
If l = 1, then M_l can be equal to -1, 0, or 1.

If l = 2, then M_l can be equal to -2, -1, 0, 1, or 2.

If l = 3, then M_l can be equal to -3, -2, -1, 0, 1, 2, or 3.

Electron Spin (M_s)

- Electrons behave as if they were spinning around an axis, much as the earth spins daily. However, unlike the earth an electron is free to spin in any direction along the axis. Thus, in turn proposing that an electron can have either of two spin values, 1/2 which is normally represented by a ↑ or -1/2 which is represented by a ↓. Electron spin numbers are not in any relation to n, l, and M_l. It is an independent number and characteristic.



Electrons will spin in opposite directions if contained in the same orbital. They spin as if they were tiny charges spheres spinning around an axis.

Pauli Exclusion Principal

Originated by Austrian physicist Wolfgang Pauli (1900-1958), no two electrons in an atom can have the same four quantum numbers. Meaning, that the quantum number for an electron is unique, like a “fingerprint” and no two electron will have the same “fingerprint.”

Pauli exclusion principal: “No two electrons in an atom have the same four quantum numbers”

Pauli Exclusion Principal vs. Electron Spin

All electrons in the same orbital must have the same values for the three quantum numbers: n, l, and M_l. In order to fulfil the Pauli Exclusion Principal the fourth quantum numbers must be different. Within each two electron carrying orbital, if the electrons have different spins (1/2 and -1/2) the Pauli Exclusion Principal is put into effect and proved true.

Example

Give a possible set of quantum numbers in a Zr atom.

1st Step: Determine what energy level Zr is located in by counting from the top of the Periodic table to the bottom.

$n = 5$

2nd Step: Determine which sublevel Zr is located. Either s, p, d, or f

$$l = 2$$

3rd Step: Give the appropriate M_l *according to the Angular-momentum Quantum Number. Either -2, -1, 0, 1, or,2.*

$$M_l = -2$$

4th Step: Assign the proper Magnetic Spin Number. Either 1/2 or -1/2.

$$M_s = 1/2$$

Therefore a possible set of Quantum Numbers for Zr is:

$n = 5$

$l = 2$

$M_l = -2$

$M_s = 1/2$

or

$n = 5$

$l = 2$

$M_l = -2$

$M_s = -1/2$

Summary of First 4 Shells

n	l	m_l	Orbital Notation	Number of Orbitals in Subshell	Number of Orbitals in Shell
1	0	0	1*s*	1	1
2	0	0	2*s*	1	4
	1	−1, 0 +1	2*p*	3	
3	0	0	3*s*	1	9
	1	−1, 0 +1	3*p*	3	
	2	−2, −1, 0 +1, +2	3*d*	5	
4	0	0	4*s*	1	16
	1	−1, 0 +1	4*p*	3	
	2	−2, −1, 0 +1, +2	4*d*	5	
	3	−3, −2, −1, 0 +1, +2, +3	4*f*	7	